MATERIAL SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

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SRM Number: 1493
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SRM Name: Polychlorinated Biphenyl Congeners in 2,2,4-Trimethylpentane

Date of Issue: 17 September 2004

Emergency Telephone ChemTrec:
1-800-424-9300 (North America)
+1 703 527 3887 (International)

Description: This Standard Reference Material (SRM) is a solution of 20 polychlorinated biphenyl (PCB) congeners in 2,2,4-trimethylpentane (isooctane). This SRM is intended primarily for use in the calibration of chromatographic instruments used for the determination of the certified compounds. A unit of SRM 1493 consists of five 2-mL ampoules, each containing approximately 1.2 mL of solution.

Substance: Polychlorinated Biphenyl Congengers in Trimethylpentane

Other Designations: **2,2,4-Trimethylpentane** (isooctane; isobutyltrimethylmethane; trimethylpentane; iso-octane; 2,2,4-trimethylpentane)

1. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Hazardous Component	CAS Number	EC Number[(a)] (EINECS)	Proportion[(b)]
2,2,4-trimethylpentane	**540-84-1**	**208-759-1**	**≈ 100 %**
2,4'-dichlorobiphenyl	33284-50-3	Not assigned	
2,2',5-trichlorobiphenyl	37680-65-2	Not found	
2,4,4'-trichlorobiphenyl	7012-37-5	230-293-2	
2,2',3,5'-tetrachlorobiphenyl	41464-39-5	Not found	
2,2',5,5'-tetrachlorobiphenyl	35693-99-03	Not found	
2,3',4,4'-tetrachlorobiphenyl	32598-10-0	Not found	
3,3',4,4'-tetrachlorobiphenyl	32598-13-3	Not assigned	
2,3',4,4',5-pentachlorobiphenyl	37680-73-2	Not found	
2,3,3',4,4'-pentachlorobiphenyl	32598-14-4	Not found	
2,3',4,4',5-pentachlorobiphenyl	31508-00-6	Not found	
3,3',4,4',5-pentachlorobiphenyl	57465-28-8	Not found	
2,2',3,3',4,4'-hexachlorobiphenyl	38380-07-3	Not found	
2,2',3,4,4',5'-hexachlorobiphenyl	35065-28-2	Not assigned	
2,2',4,4',5,5'-hexachlorobiphenyl	35065-27-1	Not assigned	
2,2',3,3',4,4',5-heptachlorobiphenyl	35065-30-6	Not found	
2,2',3,4,4',5,5'-heptachlorobiphenyl	35065-29-3	Not assigned	
2,2',3,4',5,5',6-heptachlorobiphenyl	52663-68-0	Not found	
2,2',3,3',4,4',5,6-octachlorobiphenyl	52663-78-2	Not found	
2,2',3,3',4,4',5,5',6-nonachlorobiphenyl	40186-72-9	Not found	
2,2',3,3',4,4',5,5',6,6'-decachlorobiphenyl	2051-24-3	Not found	
2,2,4-trimethylpentane	**540-84-1**	**208-759-1**	**< 100 %**

[(a)]EC Number (EINECS) not found in source(s) used.

[(b)]This material contains polychlorinated biphenyl congeners, many of which have been reported to have toxic, mutagenic, and/or carcinogenic properties, and should be handled with care. The polychlorinated biphenyl congeners in this material have a total concentration of < 0.1 % and **DO NOT** require individual MSDS information under current regulations. For actual concentrations, see the corresponding Certificate of Analysis.

Trimethylpentane	
EC Class:	F, Xn, Xi, N;
EC Risk (R No.):	R11, R38, R50/53, R65, R67
EC Safety (S No.):	S2, S9, S16, S29, S33, S60, S61, S62
See section 15:	"Regulatory Information".

3. HAZARDS IDENTIFICATION

Major Health Hazards:	Central nervous system depression. Respiratory tract irritation. Aspiration hazard.
Potential Health Effects	
Eye Contact:	Irritation may occur.
Skin Contact:	Contact may cause irritation with redness. If sufficient amounts are absorbed, systemic toxicity may occur.
Inhalation:	Exposure to trimethylpentane may cause irritation of the mucous membranes. Exposure may cause rapid breathing, dizziness, fatigue, headache, light-headedness, lack of coordination, nausea, narcosis, and other central nervous system effects. Extreme exposure may cause unconsciousness and respiratory arrest.
Ingestion:	Lung damage may occur if aspirated into the lungs and may be fatal. Symptoms may include coughing, difficulty breathing, cyanosis, and pulmonary edema. May cause diarrhea, difficulty breathing, fatigue and slight central nervous system depression. In animal studies, aspiration of C6-C8 hydrocarbons resulted in almost immediate death due to respiratory paralysis, asphyxia, and cardiac arrest.
Additional Toxicological Information:	Refer to Section 11, "Toxicological Information".
Target Organs:	Central nervous system.
Medical Conditions Aggravated by Exposure:	None reported.
Physical Hazards:	Flammable.
Additional Information on Fire and Explosion Hazards:	Refer to Section 10, "Stability and Reactivity".
Additional Toxic Information:	See section 11, "Toxicological Information".

Listed as a Carcinogen/

Potential Carcinogen:

Yes	No	
	X	In the National Toxicology Program (NTP) Report on Carcinogens.
	X	In the International Agency for Research on Cancer (IARC) Monographs.
	X	By the Occupational Safety and Health Administration (OSHA).

4. FIRST AID MEASURES

Skin Contact:	Remove contaminated clothing and shoes. Wash skin with soap and water for at least 15 minutes. Obtain medical assistance, if needed. Clean contaminated clothing before reuse.
Eye Contact:	Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Obtain medical assistance.
Inhalation:	If adverse effects occur, remove to uncontaminated area. If not breathing, give artificial respiration by qualified personnel. Get immediate medical attention.
Ingestion:	If a large amount is swallowed, obtain immediate medical assistance.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards:	This material is a severe fire hazard; the vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. Vapor/air mixtures are explosive above flash point.

Extinguishing Media:	Use extinguishing media that is compatible for the surrounding material and fire.
Fire Fighting:	Move container from fire area if possible without exposure to risk. Avoid inhalation of material or combustion by-products. As in any fire, wear full protective clothing and NIOSH-approved self-contained breathing apparatus.
Flash Point (°C):	-12 °C
Method Used:	CC
Autoignition Temp. (°C):	415 °C
Flammability Limits in Air	
Upper (Volume %):	6.0
Lower (Volume %):	1.1

6. ACCIDENTAL RELEASE MEASURES

Occupational Release:	Isolate the hazard area and deny entry. Collect spilled material in appropriate container for disposal. Keep out of water supplies and sewers.
Disposal:	See section 13, "Disposal Considerations".

7. HANDLING AND STORAGE

Storage:	Store and handle in accordance with all current regulations and standards. Store material with the cap tightly closed, in a dry environment, and under normal laboratory conditions. Keep separated from incompatible materials.
Safe Handling Precautions:	Use methods to minimize dust. See section 8, "Exposure Controls and Personal Protection".

8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

Occupational Exposure Limits:	**Trimethylpentane** No occupational limits established.
Engineering:	An eye wash station, drench shower, and a local exhaust ventilation system should be readily available near areas of use.
Ventilation:	Use a local exhaust ventilation system. Ensure compliance with applicable exposure limits.
Respirator:	For conditions of frequent use or heavy exposure where exposure is apparent and engineering controls are not feasible, respirator protection may be needed. Refer to the "NIOSH Guide to the Selection and Use of Particulate Respirators Certified under 42 CFR 84" for selection and use of respirators certified by NIOSH.
Eye Protection:	Wear safety goggles. **DO NOT** wear contact lenses in the laboratory.
Clothing:	Wear appropriate protective clothing to prevent skin exposure.

9. PHYSICAL AND CHEMICAL PROPERTIES

Component:	**2,2,4-Trimethylpentane**
Appearance and Odor:	Clear liquid. Gasoline odor.
Molecular Weight:	114.23
Molecular Formula:	$(C\text{-}H_3)_2\text{-}C\text{-}H\text{-}C\text{-}H_2\text{-}C\text{-}(C\text{-}H_3)_3$
Specific Gravity:	0.6919 g/cm^3
Boiling Point:	99 °C
Water Solubility:	Immiscible.
Solvent Solubility:	Soluble in ether, alcohol, acetone, benzene, toluene, chloroform, xylene, carbon disulfide, carbon tetrachloride, dimethylformamide, oils

10. STABILITY AND REACTIVITY

Stability: X **Stable** _____ **Unstable**

Stable at normal temperatures and pressure.

Conditions to Avoid: None reported.

Incompatible Materials: Trimethylpentane is incompatible with metals and oxidizing materials

See Section 5: "Fire Fighting Measures".

Hazardous Decomposition: Thermal decomposition of trimethylpentane may produce oxides of carbon.

Hazardous Polymerization: _____ **Will Occur** X **Will Not Occur**

11. TOXICOLOGICAL INFORMATION

Route of Entry: X **Inhalation** X **Skin** X **Ingestion**

Toxicological Data

Rat, Inhalation LC_{50}: 33.52 mg/15 min

Rat, Oral LD_{50}: > 5000 mg/kg

Target Organs: Central nervous system.

Medical Conditions Aggravated by Exposure: None known.

Health Effects (Acute and Chronic): See section 3, "Hazards Identification," for potential health effects.

12. ECOLOGICAL INFORMATION

Ecotoxicity Data: Not available.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with all applicable federal, state, and local regulations. Keep out of water supplies and sewers.

14. TRANSPORTATION INFORMATION

U.S. DOT and IATA: Octanes; Class Hazard 3; Packing Group II; ID No. UN1262.

15. REGULATORY INFORMATION

U.S. REGULATIONS:

SARA TITLE III SARA SECTIONS 311/312 HAZARDOUS CATEGORIES (40 CFR 370.21):

ACUTE:	Yes
CHRONIC:	No
FIRE:	Yes
REACTIVE:	No
SUDDEN RELEASE:	No

EC CLASSIFICATION:

F	Highly Flammable
Xn	Harmful
Xi	Irritant
N	Dangerous for the Environment

EC RISK AND SAFETY PHRASES:

R11	Highly flammable.
R38	Irritating, to skin.
R50/53	Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
R65	Harmful: may cause lung damage if swallowed.
R67	Vapors may cause drowsiness and dizziness.
S2	Keep out of reach of children
S9	Keep container in a well-ventilated place.
S16	Keep away from sources of ignition - No smoking.
S29	Do not empty into drains.
S33	Take precautionary measures against static discharges.
S60	This material and/or its container must be disposed of as hazardous waste.
S61	Avoid release to the environment. Refer to special instructions/Safety data sheets.
S62	If swallowed, do not induce vomiting: seek medical advice immediately and show this container or label.

16. OTHER INFORMATION

Sources: MDL Information Systems, Inc., MSDS *2,2,4-Trimethylpentane,* 19 March 2003.

Certificate 1493 *Polychlorinated Biphenyl Congeners in 2,2,4-Trimethylpentane*; National Institute of Standards and Technology, U.S. Department of Commerce: Gaithersburg, MD (1995).